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Analysis of the dynamics of liquid aluminium: Recurrent relation approach

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Abstract

By use of the recurrent relation approach (RRA) we study the microscopic dynamics of liquid aluminium at T ≤ 973K and develop a theoretical model which satisfies all the corresponding sum rules. The investigation covers the inelastic features as well as the crossover of our theory into the hydrodynamical and the free-particle regimes. A comparison between our theoretical results with those following from a generalized hydrodynamical approach is also presented. In addition to this we report the results of our molecular dynamics simulations for liquid aluminium, which are also discussed and compared to experimental data. The results obtained reveal (i) that the microscopical dynamics of density fluctuations is defined mainly by the first four even frequency moments of the dynamic structure factor, and (ii) the inherent relation of the high-frequency collective excitations observed in experimental spectra of dynamic structure factor S(k,ω) with the two-, three-and four-particle correlations.

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